

Iridium double perovskite Sr₂YIrO₆: A combined structural and specific heat study

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Abstract

© 2017 American Physical Society. Recently, the iridate double perovskite Sr₂YIrO₆ has attracted considerable attention due to the report of unexpected magnetism in this Ir⁵⁺ (5d⁴) material, in which according to the Jeff model, a nonmagnetic ground state is expected. However, in recent works on polycrystalline samples of the series Ba_{2-x}Sr_xYIrO₆ no indication of magnetic transitions have been found. We present a structural, magnetic, and thermodynamic characterization of Sr₂YIrO₆ single crystals, with emphasis on the temperature and magnetic field dependence of the specific heat. As determined by x-ray diffraction, the Sr₂YIrO₆ single crystals have a cubic structure, with space group Fm $\bar{3}$ m. In agreement with the expected nonmagnetic ground state of Ir⁵⁺ (5d⁴) in Sr₂YIrO₆, no magnetic transition is observed down to 430 mK. Moreover, our results suggest that the low-temperature anomaly observed in the specific heat is not related to the onset of long-range magnetic order. Instead, it is identified as a Schottky anomaly caused by paramagnetic impurities present in the sample, of the order of $n \sim 0.5(2)\%$. These impurities lead to non-negligible spin correlations, which nonetheless, are not associated with long-range magnetic ordering.

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References

- [1] J. G. Rau, E. Kin-Ho Lee, and Hae-Young Kee, *Annu. Rev. Condens. Matter Phys.* **7**, 195 (2016). 1947-5454 10.1146/annurev-conmatphys-031115-011319
- [2] W. Witczak-Krempa, G. Chen, Y. Baek Kim, and L. Balents, *Annu. Rev. Condens. Matter Phys.* **5**, 57 (2014). 1947-5454 10.1146/annurev-conmatphys-020911-125138
- [3] A. Nag, *Phys. Rev. Lett.* **116**, 097205 (2016). PRLTAO 0031-9007 10.1103/PhysRevLett.116.097205
- [4] S. Chikara, O. Korneta, W. P. Crummett, L. E. DeLong, P. Schlottmann, and G. Cao, *Phys. Rev. B* **80**, 140407 (R) (2009). PRBMDO 1098-0121 10.1103/PhysRevB.80.140407
- [5] M. Ge, T. F. Qi, O. B. Korneta, D. E. De Long, P. Schlottmann, W. P. Crummett, and G. Cao, *Phys. Rev. B* **84**, 100402 (R) (2011). PRBMDO 1098-0121 10.1103/PhysRevB.84.100402
- [6] Y. Chen and H. Y. Kee, *Phys. Rev. B* **90**, 195145 (2014). PRBMDO 1098-0121 10.1103/PhysRevB.90.195145
- [7] G. Jackeli and G. Khaliullin, *Phys. Rev. Lett.* **102**, 017205 (2009). PRLTAO 0031-9007 10.1103/PhysRevLett.102.017205
- [8] D. Pesin and L. Balents, *Nat. Phys.* **6**, 376 (2010). 1745-2473 10.1038/nphys1606
- [9] X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, *Phys. Rev. B* **83**, 205101 (2011). PRBMDO 1098-0121 10.1103/PhysRevB.83.205101
- [10] W. Witczak-Krempa and Y. B. Kim, *Phys. Rev. B* **85**, 045124 (2012). PRBMDO 1098-0121 10.1103/PhysRevB.85.045124

- [11] A. A. Burkov and L. Balents, *Phys. Rev. Lett.* 107, 127205 (2011). PRLTAO 0031-9007 10.1103/PhysRevLett.107.127205
- [12] W. Witczak-Krempa, T. P. Choy, and Y. B. Kim, *Phys. Rev. B* 82, 165122 (2010). PRBMDO 1098-0121 10.1103/PhysRevB.82.165122
- [13] M. Kargarian, J. Wen, and G. A. Fiete, *Phys. Rev. B* 83, 165112 (2011). PRBMDO 1098-0121 10.1103/PhysRevB.83.165112
- [14] X. Wan, A. Vishwanath, and S. Y. Savrasov, *Phys. Rev. Lett.* 108, 146601 (2012). PRLTAO 0031-9007 10.1103/PhysRevLett.108.146601
- [15] A. Go, W. Witczak-Krempa, G. S. Jeon, K. Park, and Y. B. Kim, *Phys. Rev. Lett.* 109, 066401 (2012). PRLTAO 0031-9007 10.1103/PhysRevLett.109.066401
- [16] N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements* (Elsevier-Butterworth-Heinemann, Amsterdam, 2012).
- [17] G. Chen, R. Pereira, and L. Balents, *Phys. Rev. B* 82, 174440 (2010). PRBMDO 1098-0121 10.1103/PhysRevB.82.174440
- [18] B. J. Kim, *Phys. Rev. Lett.* 101, 076402 (2008). PRLTAO 0031-9007 10.1103/PhysRevLett.101.076402
- [19] M. Wakeshima, D. Harada, and Y. J. Hinatsu, *J. Alloys Compd.* 287, 130 (1999). JALCEU 0925-8388 10.1016/S0925-8388(99)00057-2
- [20] G. Cao, T. F. Qi, L. Li, J. Terzic, S. J. Yuan, L. E. DeLong, G. Murthy, and R. K. Kaul, *Phys. Rev. Lett.* 112, 056402 (2014). PRLTAO 0031-9007 10.1103/PhysRevLett.112.056402
- [21] S. Bhowal, S. Baidya, I. Dasgupta, and T. Saha-Dasgupta, *Phys. Rev. B* 92, 121113 (R) (2015). PRBMDO 1098-0121 10.1103/PhysRevB.92.121113
- [22] K. Pajskr, P. Novák, V. Pokorný, J. Kolorenč, R. Arita, and J. Kuneš, *Phys. Rev. B* 93, 035129 (2016). 2469-9950 10.1103/PhysRevB.93.035129
- [23] B. Ranjbar, E. Reynolds, P. Kayser, and B. J. Kennedy, *Inorg. Chem.* 54, 10468 (2015). INOCAJ 0020-1669 10.1021/acs.inorgchem.5b01905
- [24] B. F. Phelan, E. M. Seibel, D. Badoe, Jr., W. Xie, and R. J. Cava, *Solid State Commun.* 236, 37 (2016). SSCOA4 0038-1098 10.1016/j.ssc.2016.03.017
- [25] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevB.95.064418> for anisotropic displacement parameters and selected bond lengths and angles.
- [26] Bruker, computer code apex2 Software Suite for Crystallographic Programs, Bruker AXS Inc., Madison, WI, 2009.
- [27] Bruker, computer code Area Detector Control and Integration Software, Version 5.x. In smart and saint, Bruker AXS Inc., Madison, WI, 1996.
- [28] G. M. Sheldrick, *Acta Crystallogr. Sect. A* 64, 112 (2008). ACACEQ 0108-7673 10.1107/S0108767307043930
- [29] G. M. Sheldrick, computer code cell now, program for unit cell determination, University of Göttingen, Germany, 2005 and Bruker AXS Inc., Madison, WI, 2005.
- [30] G. M. Sheldrick, computer code twinabs, Bruker AXS scaling for twinned crystals, Version 2007/3, and sadabs, University of Göttingen, Germany, 2007 and Bruker AXS Inc, Madison WI, 2007.
- [31] A. L. Spek, *Acta Crystallogr. Sect. D* 65, 148 (2009). ABCRE6 0907-4449 10.1107/S090744490804362X
- [32] A.-C. Dippel, H.-P. Liermann, J. T. Delitz, P. Walter, H. Schulte-Schrepping, O. H. Seeck, and H. Franz, *J. Synchrotron Radiat.* 22, 675 (2015). 1600-5775 10.1107/S1600577515002222
- [33] H. M. Rietveld, *J. Appl. Crystallogr.* 2, 65 (1969). JACGAR 0021-8898 10.1107/S0021889869006558
- [34] T. Roisnel and J. Rodríguez-Carvajal, *Mater. Sci. Forum* 378-381, 118 (2001). 10.4028/www.scientific.net/MSF.378-381.118
- [35] T. Dey, *Phys. Rev. B* 93, 014434 (2016). 2469-9950 10.1103/PhysRevB.93.014434
- [36] M. Bremholm, S. E. Dutton, P. W. Stephens, and R. J. Cava, *J. Solid State Chem.* 184, 601 (2011). JSSCBI 0022-4596 10.1016/j.jssc.2011.01.028
- [37] Note that the tiny humps in the 5-T curve are due to technical artifacts which are arising from the combination of the large number of data points and negligible changes in the susceptibility in the shown temperature regime.
- [38] P. Kayser, M. J. Martínez-Lope, J. A. Alonso, M. Retuerto, M. Croft, A. Ignatov, and M. T. Fernández-Díaz, *Inorg. Chem.* 52, 11013 (2013). INOCAJ 0020-1669 10.1021/ic401161d
- [39] A Brillouin function with (Equation presented) also allows to fit the data. However, this fit leads to unphysical (Equation presented) values.
- [40] Y. Du, Z. X. Cheng, S. X. Dou, X. L. Wang, H. Y. Zhao, and H. Kimura, *Appl. Phys. Lett.* 97, 122502 (2010). APPLAB 0003-6951 10.1063/1.3490221
- [41] C. G. F. Blum, *J. Cryst. Growth* 421, 39 (2015). JCRGAE 0022-0248 10.1016/j.jcrysgro.2015.04.004

- [42] Y. Cai, Y. Li, and J. Cheng, in *Perovskite Materials-Synthesis, Characterisation, Properties, and Applications* (InTech, Rijeka, 2016).